

# DEVELOPMENT OF MATHEMATICAL MODEL FOR AN ADIABATIC OPERATION ON BIO-DEGRADATION OF PETROLEUM HYDROCARBON IN A PLUG FLOW REACTOR

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## Abstract

In this paper mathematical models were developed to simulate the plug flow reactor dimensions for an adiabatic operation on biodegradation of petroleum hydrocarbon. Computations were made on reactor volume, length, space time, and space velocity. Results obtained showed that changes in biomass growth rate and substrate concentration were observed with respect to reactor volume, length, space time and space velocity for the various theories postulated by Eckenfelder, Mosers, Miura's and Monod. Results obtained from the investigation showed that Eckenfelders model is more reliable and gives more accurate results in terms of reactor dimensions and as well as functions of biomass growth rate and substrate concentration. The developed models are useful in monitoring and predicting the petroleum hydrocarbon degradation in a plug flow reactor for adiabatic process.

**Keywords:** Adiabatic, biodegradation, petroleum hydrocarbon, model simulation.

## Introduction

In chemical engineering, physical operations such as heat transfer, mass transfer, fluid flow and separation processes are very essential and these processes play very important roles in the manufacturing firm. In the society today, there is great demand for chemical and petrochemical products. Considering the development of methodical model for an adiabatic operation on biodegradation of petroleum hydrocarbon in a plug flow reactor becomes very necessary to the chemical engineers (Vogel & Ott, 2007; Echoscans 2006; Koga, Berg, & Humphrey 1967; Harms, & Bosnia 1997).

To minimize the problem that arises from the acute degradation of petroleum hydrocarbon, there is need to develop a mathematical model that will predict the biodegradation rate, microbial growth rate, space time, space velocity, length of reactor, diameter of reactor and volume of reactor for a simple plug flow reactor system.

Several investigations conducted revealed that biodegradation reduces waste on a contaminated environment as well as enhanced environmental clean-up<sup>[6,13]</sup>. Biodegradation could be defined as the nature's way of recycling waste or breaking down organic matter into nutrient that can be used by other organisms as a source of energy (Lilovitz, Schmitz & Holm 1988; Wikipedia 2006; Gerardet, Murray, Cstillion, Nester, Wood, Krieg & Philips 1981, Brakstad & Bonaunet 2006 Bade, Taussing & Marks 2000). Some organic matter taken longer time to decay than others (Ott 2007; Ukpaka, Ogoni, Amadi & Adebayo 2004; Kinigoma 2002). Biodegradation is an effective, economical and environmentally friendly method in which microbes are used to degrade, petroleum hydrocarbons by either bioaugmentation (this is a process whereby cultured micro organisms are introduced into a contaminated system), or biostimulation (this is a process whereby additional nutrients are introduced primarily as fertilizers to stimulate microbial growth (Renneboog 2006; Sarkar, Datta & Ferguson 2003; Ophardt, 2003).

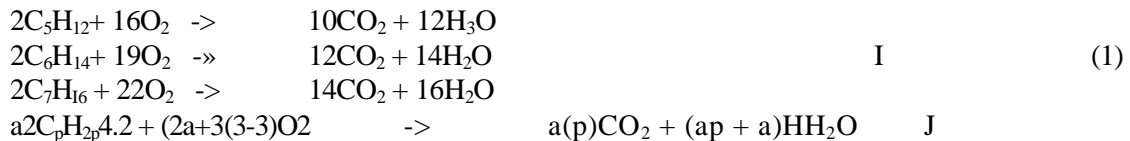
Adiabatic process involves no heat in the system, that is no heat energy is allowed to cross the boundary. In other words, in adiabatic operation no heat energy comes in or goes out of the system (Aiba, Haung, Moritz & Someya (1969).

In the present paper, an attempt to describe the effect of adiabatic operation on biodegradation of petroleum hydrocarbon in a plug flow reactor based the various model developed by different research groups such as; Eckenfelder, Mosers, Mi lira's and Mond-model. The developed models by the various research groups were modified in this paper by considering

the reactor to be a plug flow as well as reaction under adiabatic process. A few investigators have experimentally used a plug flow bioreactor for examining the degradation of various contaminants. But no realistic model has been developed to correlate the functional parameters as a major factor on biodegradation of petroleum hydrocarbon for an adiabatic process; putting into consideration the different models developed by various scientists.

### The Model

In the case of oxidation of petroleum hydrocarbon, a plug flow reactor was used and the various reaction mechanisms involved are given as;



Q is positive when heat is added to the system. Conversely, when Q is negative, heat is being given off by the system to the surroundings. Therefore, considering the case in which the reactor volume is insulated from the surroundings and the reaction shown above can be written as



Takes place adiabatically (Q = 0)

The Biochemical kinetics of the system from equation (I) can be expressed by considering the following realistic assumptions such as;

- (a) The oxidation of petroleum hydrocarbon under adiabatic process is a first order reaction.
- (b) It is assumed that the reactions above are elementary reaction i.e. first order elementary reaction.
- (c) The reactions above have been considered to be a bio-oxidation reactions.
- (d) The system is in the liquid phase
- (e) Reactions are assumed to be independent of one another and interdependent on each other.
- (f) It is assumed that only CO<sub>2</sub> and H<sub>2</sub>O are produced.

### The Kinetic Model for Petroleum Hydrocarbon

The Arrhenius equation is given as

$$K_s = A_0 V^{\Delta L}$$

The rate expression can be written as

$$-r_A = \frac{K_s C_A C_B}{1 + K_A C_A + K_B C_B} \tag{3}$$

where C<sub>A</sub> is concentration of the individual petroleum hydrocarbon C<sub>B</sub> is concentration of oxygen.

Also the mole fraction X<sub>A</sub> is given as:

$$X_A = \frac{C_{AO} - C_A}{C_{AO}}$$

Similarly  $X_B = \frac{C_{BO} - C_B}{C_{BO}}$

Here  $X_A C_{AO} = C_{AO} - C_A$

$$C_A = (1 - X_A) C_{AO}$$

Similarly  $C_B = (1 - X_B) C_{BO}$

From stoichiometry

$$\frac{X_A C_{AO}}{1} = \frac{C_{AO} X_A - C_A}{1}$$

From stoichiometry

$$\frac{X_A C_{AO}}{2} = \frac{C X_B - C_{BO}}{2\alpha + 3\beta - 3}$$

Or

$$\frac{X_A C_{AO}}{\alpha} = \frac{C_B - C_{BO}}{2\alpha + 3\beta - 3}$$

where  $\alpha = 2$ , and  $\beta = 1, 2, 3, 4, 5, 6, 7, 8$  —etc. Hence from equation (9)

$$X_B = \frac{X_A (2\alpha + 3\beta - 3) C_{AO}}{\alpha C_{BO}}$$

Equation (10) can also be written as

$$X_B = \frac{X_A (2\alpha + 3\beta - 3)}{\alpha} \left( \frac{C_{AO}}{C_{BO}} \right)$$

$$\text{Let } \phi = \frac{C_{AO}}{C_{BO}} \text{ and } \psi = \frac{C_{BO}}{C_{AO}}$$

(4) (5)

(6)

(7) (8) (9)

(10) CO

For paraffinic compound with  $C_n H_{2n+2}$ , where  $p = 5$ , therefore, equation (11) becomes

$$X_B = \frac{X_A (2 * 2 + 3(5) - 3)}{2} \left( \frac{C_{AO}}{C_{BO}} \right)$$

$$X_B = 8 X_A \frac{C_{AO}}{C_{BO}} \quad \text{for pentane} \quad (12)$$

Therefore substituting equations (6 and?) into equation (3) yields.

$$C_{AO} \frac{dX_A}{dt} = (-R_A) = K_1 C_{AO} (1 - X_A) C_{BO} (1 - X_B) \quad (13)$$

Substituting equation (12) into equation (13) yields

$$C_{AO} \frac{dX_A}{dt} = (-R_A) = K_1 C_{AO} (1 - X_A) C_{BO} \left( 1 - 8 X_B \frac{C_{AO}}{C_{BO}} \right) \quad (14)$$

$$C_{AO} \frac{dX_A}{dt} = (-R_A) = K_1 C_{AO} (1 - X_A) C_{BO} (1 - 8 X_B \phi) \quad (15)$$

Therefore

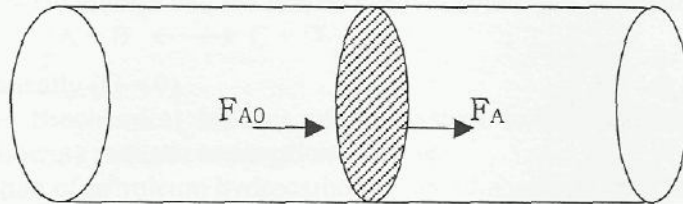
$$\frac{dX_A}{dt} = (-R_A) = K_1 (1 - X_A) \frac{C_{BO}}{C_{AO}} (1 - 8 X_B \phi) \quad (36)$$

$$\frac{dX}{dt} = (-R_A) = K_1 (1 - X_A) \psi (1 - 8 X_A \phi) \quad (17)$$

### The Plug Flow Model

Bioremediation operations can be carried out in a plug flow reactor. The research work was conducted in a plug flow reactor as shown in the project work. Therefore applying the basic principle laws of conservation of mass, energy and momentum and taking the component material balance for the given process is given as

$$\left[ \begin{array}{l} \text{Rate of input} \\ \text{of A} \end{array} \right] = \left[ \begin{array}{l} \text{Rate of output} \\ \text{of A} \end{array} \right] \pm \left[ \begin{array}{l} \text{Rate of disappearance} \\ \text{due to chemical reaction} \end{array} \right] - \left[ \begin{array}{l} \text{Rate of accumulation} \\ \text{of A in the system} \end{array} \right] \quad (18)$$



$$F_{AO} = F_A + (-R_A) V \quad (19)$$

$$\text{where } F_A = F_{AO} (1 - X_A) \quad (20)$$

$$F_{AO} = F_{AO} (1 - X_A) + (-R_A) V \quad (21)$$

$$F_{AO} = F_{AO} - F_{AO} X_A + (-R_A) V$$

$$F_{AO} X_A = (-R_A) V$$

In case where the reaction rate can be expressed as a single conversion variable X, the design equation giving the reactor volume necessary to achieve a conversion X in a tubular reaction is (23)

$$V = F_{AO} \int_0^{X_A} \frac{dX_A}{(-R_A)}$$

Equation (22) can also be written as

$$(-R_A) V = F_{AO} \int_0^{X_A} dX_A$$

$$\text{where } (-R_A) = K_1 (1 - X_A) \psi (1 - 8 X_A \phi)$$

Substituting equation (37) into equation (22) yields

$$K_1 \psi V = F_{AO} \int_0^{X_A} \frac{dX_A}{(1-X_A)(1-8X_A\phi)} \quad (24)$$

$$K_1 \psi V = F_{AO} \int_{AO}^{X_A} \frac{dX}{(1-X_A)(1-8X_A\phi)} \quad (25)$$

Integrating equation (24) yields

$$\frac{K_1 \psi V}{F_{AO}} = \ln \frac{1-8\phi X_A}{1-X_A} \quad (26)$$

Therefore

$$\frac{1-8\phi X_A}{1-X_A} = \lambda^{\frac{K_1 \psi V}{F_{AO}}}$$

### Kinetic Models for Microbial Growth

The affinity of a microorganism for hydrocarbons determines the mode of uptake of the hydrocarbons. Based on this affinity, several models have been proposed for hydrocarbon-degrading microbes. Generally, the models appear to be modified versions of the Monod-type equation given as

$$\frac{1}{X} \frac{dX}{dt} = \mu = \frac{\mu_{\max} \cdot S}{K_s + S} \quad (27)$$

where X is cell concentration; t is time, S is-substrate concentration, K<sub>s</sub> is the saturation constant while U- and u<sub>max</sub> are the specific growth rate and the maximum specific growth rate respectively.

For microorganism with low affinity for liquid hydrocarbon Aiba, Haung, Moritz & Someya (1969), on the assumption that the most susceptible oil drops to microbial uptake are in "accommodation" form, proposed the model.

$$\mu = \frac{\mu_{\max} S^*}{K_s + S^*} \quad (28)$$

Where S\* is the concentration of accommodated oil which can be obtained from a correlation with, operating conditions; u., u<sub>max</sub> and K<sub>s</sub> are as defined earlier. Moo-young and Shimizu (1971) proposed Monod-type equation for microorganisms with high affinity

$$\mu = \frac{\mu_{\max} P}{K_p + P} \quad (29)$$

For hydrocarbons where the  $\frac{\mu_{\max} P}{K_p + P}$  governed by the extent of the probable cell attachment to the surface ("drop", form), P is the number of cells per unit volume of dispersion which can be attached to the droplets while K<sub>p</sub> is the saturation constant for the potential P. Also Miura (1978) proposed a model of the type for organism with high affinity for liquid

$$\mu = \frac{\mu_{\max} S/X}{K_s + S/X} \quad (30)$$

Hydrocarbons: All the parameters are as defined earlier but may be noted that S/X is the specific concentration of hydrocarbon per unit cell mass in the medium. Inherent in this model is the assumption that such organism creates a hydrocarbon pool in/or on the cell.

Analogous to chemical reaction, if the biomass (cell) represent the product or one of the products of the reaction and hydrocarbon the reactant, kinetic models can also be written based on the specific rate of substrate (hydrocarbon) assumption, r<sub>s</sub>. Monod-type based on substrate consumption i.e.

$$\eta_s = -\frac{1}{X} \frac{dS}{dt} = \frac{\eta_{s \max} S}{K_s + S} \quad (31)$$

Has actually been used in waste treatment processes as reported (Miura 1978), other such models used in waste treatment include Eckenfelder's model as reported by Miura (1978).

$$\eta_s = K \cdot S \quad (32)$$

and Moser's model as presented (Miura 1978)

$$\eta_s = \frac{\eta_{s \max} S^2}{K_s^2 + S^2} \quad (33)$$

Where  $K$  is a constant approximately equal to  $\frac{\eta_{s \max}}{K_s}$  and  $K_s$  is the saturation constants,  $\eta_{s \max}$  is the maximum specific substrate consumption rate and other parameter are as already defined.

Based on the above, an adapted Miura's model of the form may be considered here in describing the

$$\eta_s = \frac{\eta_{s \max} S / X}{K_s + S / X} \quad (34)$$

high affinity for liquid hydrocarbons.

In this work, this model i.e. equation (34); Monod-type model (equation 31), Eckenfelder's model (equation 32) and Moser's model (equation 33) were tested to ascertain their fit of the acquired data and thus determine the applicable kinetic model that describe the mechanisms of hydrocarbon uptake by the organism in the development of mathematical model for an adiabatic operation on biodegradation of petroleum hydrocarbon in a plug flow reactor.

#### Model for Microbial Heat Generation (Q)

The instantaneous microbial heat generation rate  $Q_g$  is given as

$$Q_{mHG} = V_{reactor} \sigma \eta \frac{1}{Y_\Delta} \quad (35)$$

Substituting equation (27) into 35) yields the expression in terms of Monod-type of microbial heat generation in the system.

$$Q_{mm} = V_{reactor} \sigma \frac{\mu_{\max} \cdot S}{K_s + S} \cdot \frac{1}{Y_\Delta} \quad (36)$$

mm = Monod model

where  $\mu$  = specific growth rate

In terms of low affinity for liquid hydrocarbon

$$Q_{mmL} = V_{reactor} \sigma \frac{\mu_{\max} S^*}{K_s + S^*} \cdot \frac{1}{Y_\Delta} \quad (37)$$

mmL = Monod model for low affinity

In terms of high affinity for liquid hydrocarbon (Product formation).

$$Q_{mmHP} = V_{reactor} \sigma \frac{\mu_{\max} P}{K_p + P} \cdot \frac{1}{Y_\Delta} \quad (38)$$

mmHP = Monod model for high affinity of product formed

$$Q_{mmHS} = V_{reactor} \sigma \frac{\mu_{\max} S / X}{K_p + S / X} \cdot \frac{1}{Y_\Delta} \quad (39)$$

MMHS = Monod model for high affinity of specific growth rate.

Similarly, since  $\eta_s = -\frac{1}{X} \frac{dS}{dt} = \frac{\eta_{s \max} S}{K_s + S}$

Equation (35) can be written as

$$Q = V_{\text{reactor}} \sigma \left( \frac{-1}{X} \frac{dS}{dt} \right) \frac{1}{Y_A} = V_{\text{reactor}} \sigma \frac{\eta_{s \max} S_1}{K_s + S Y_\Delta} \quad (40)$$

Expressing the microbial heat generated in the system based on Eckenfelder's model yields

$$Q_{ECM} = V_{\text{reactor}} \sigma K.S. \frac{1}{Y_\Delta} \quad (41)$$

In terms of Moser's model

$$Q_{mom} = V_{\text{reactor}} \sigma \frac{\eta_{s \max} S^2}{K_s^2 + S^2} \frac{1}{Y_\Delta} \quad (42)$$

and finally, in terms of Miura's model

$$Q_{min} = V_{\text{reactor}} \sigma \frac{\eta_{s \max} S/X}{K_s^2 + S/X} \frac{1}{Y_\Delta} \quad (43)$$

The mathematical expression for  $Y_\Delta$  is given as

$$Y_\Delta = \frac{Y_s}{\Delta H_s - Y_s \Delta H_c} \left( \frac{g - \text{cell} / g \text{ substrate}}{Kcal / g \text{ substrate}} \right) \quad (44)$$

and

$$Y_s = \frac{\mu}{\frac{\mu}{Y_g} + Ke} \left( \frac{g \text{ cell}}{g \text{ substrate consumed}} \right) \quad (45)$$

$$Y_\Delta = \frac{\mu^2 Y_s}{\mu \Delta H_s - Y_g (\mu \Delta H_c - \Delta H_s Ke)}$$

Substituting equation (45) into equation (44) and making  $Y_A$  the subject of the formula yields (46)

The model was simplified based on the following

assumptions

- (a) A balance for cell combustion is written assuming the product to be CO<sub>2</sub> and H<sub>2</sub>O as shown in equation (1)
- (b) The cellular heat of combustion is AH<sub>10</sub> + per weight of "cell" for the pseudomonas species (fluorescents) is expressed as

$$\frac{4.0 \text{ mol } O_2 (m.20Kcal/mol O_2)}{2[(12)(1 + (1)4)]} \quad \text{''} \quad \overset{\wedge}{m \cdot Kra, 0} \quad \text{1 J-UZJACU// £}$$

- (c) The value of step b is corrected for ash content of cell, e.g. 10wt percent in dried cells, the heat combustion for pseudomonas fluorescents from step b is AH<sub>C</sub> = (13.025Kcal/g) (0.90) = 11,7225Kcal/g dry cell mass.
- (d) Also the following data was available in the literature for some of the characteristics of n-paraffins Abbott et al (1973).
  - (i) Yield coefficient  $Y_s = Y_g$  for cell growth on n-paraffins (carbon sources) = 1,039 cell/g of substrate.
  - (ii) Yield factor  $Y_A$  (grain of cell mas per kilocalorie of heat evolved) for

substrate and oxygen

on n-paraffins = 0.16g cell /kcal. (iii)  
n-paraffins (carbon sources) = 0.50g cell/g of O<sub>2</sub>  
consumed.

Yield coefficient (Y<sub>0</sub>) for cell growth on

Using equation (3.45) to determine the heat of combustion of a substrate (AHs) for each of the component, as shown.

$$0.16 = \frac{1.03}{\Delta H_s - 1.03 (11.7225)}$$

Therefore  $\Delta H_s = 18.5 \text{ Kcal/g}$

(e) Using Ukpaka et al (2005) value for

$$K_e = -\ln \frac{2}{3} = 0.4055$$

Substituting the values obtained from the assumptions into equation (46) yields

$$\left. \begin{aligned} Y_{\Delta} &= \frac{\mu^2}{6.1\mu - 7.5} \\ \text{Or} \\ Y_{\Delta} &= \frac{\eta^2}{6.1\eta - 7.5} \end{aligned} \right\} \quad (47)$$

Therefore equation (35) can be written as

$$Q_{\text{mlHG}} = V_{\text{reactor}} \sigma \left( \frac{6.1\eta - 7.5}{\eta} \right) \quad (48)$$

In terms of Monod model

$$Q_{\text{mm}} = V_{\text{reactor}} \sigma \frac{\mu_{\text{max}} \cdot S}{K_s + S} \left( \frac{6.1\mu - 7.5}{\mu^2} \right) \quad (49)$$

In terms of low affinity for liquid hydrocarbon

$$Q_{\text{mmL}} = V_{\text{reactor}} \sigma \frac{\mu_{\text{max}} \cdot S^*}{K_s + S^*} \left( \frac{6.1\mu - 7.5}{\mu^2} \right) \quad (50)$$

In terms of high affinity for liquid hydrocarbon (product formation)

$$Q_{\text{mmHp}} = V_{\text{reactor}} \sigma \frac{\mu_{\text{max}} \cdot P}{K_p + P} \left( \frac{6.1\mu - 7.5}{\mu^2} \right) \quad (51)$$

and

$$Q_{\text{mmHS}} = V_{\text{reactor}} \sigma \frac{\mu_{\text{max}} \frac{S}{X}}{K_s + \frac{S}{X}} \left( \frac{6.1\mu - 7.5}{\mu^2} \right) \quad (52)$$

In terms of Eckenfilders model

$$Q_{\text{ECM}} = V_{\text{reactor}} \sigma K_s S \left( \frac{6.1\mu - 7.5}{\mu^2} \right) \quad (53)$$

In terms of Mosers model

$$Q_{\text{mom}} = V_{\text{reactor}} \sigma \frac{\eta_{s\text{max}} S^2}{K_s^2 + S^2} \left( \frac{6.1\mu - 7.5}{\mu^2} \right)$$

In terms  
of  
Miura s



model

(54)

$$Q_{\text{mim}} = V_{\text{reactor}} \sigma \frac{\eta_{s \text{ max}} S/X}{K_s + S/X} \left( \frac{6.1\mu - 7.5}{\mu^2} \right) \quad (55)$$

Considering the adiabatic process of the system where  $Q_{\text{imm}0} = Q_{\text{mm}} - Q_{\text{mmi}} = Q_{\text{mmHp}} - Q_{\text{mmHS}} - Q_{\text{ficm}}$

$$0 = V_{\text{reactor}} \sigma \cdot K \cdot S \cdot \left( \frac{6.1\mu - 7.5}{\mu^2} \right)$$

Rearranging yields

$$6.1\mu \frac{V_{\text{reactor}}}{\mu^2} \sigma \cdot K \cdot S - 7.5 \frac{V_{\text{reactor}}}{\mu^2} \sigma \cdot K \cdot S = 0$$

$$6.1\mu \frac{V_{\text{reactor}}}{\mu^2} \sigma \cdot K \cdot S - 7.5 \frac{V_{\text{reactor}}}{\mu^2} \sigma \cdot K \cdot S$$

=  $Q_{\text{mom}} = Q_{\text{mim}} = 0$ , therefore equation (48), (49), (50), (51), (52), (53), (54), Bind (55) have equal

$$\mu = \frac{7.5 V_{\text{reactor}} \sigma K \cdot S \mu^2}{6.1 V_{\text{reactor}} \sigma K \cdot S \mu^2}$$

$$\mu = \frac{7.5}{6.1} = 1.23$$

value of specific rate  $u = r_i = 1.23$  considering equation (53)

Therefore // =  $r_j = 1.23$

Since reactor volume can be expressed as  
 $V_r = Ah$

Therefore equation (5,) becomes,  $i r_{Q_{11} | m | p, 0}$

$$\frac{1}{V_R} = \frac{\sigma \mu_{\text{max}} \cdot r}{K_p + P} \left( \frac{0.1\mu - 7.5}{\mu^2} \right) \quad (56)$$

$$V_R = \frac{K_p + P}{\sigma \mu_{\text{max}} P} \left( \frac{\mu^2}{6.1\mu - 7.5} \right) \quad (57)$$

Since for a cylindrical object the volume of a reactor is given as;

$$\pi r^2 l = \frac{K_p + P}{\sigma \mu_{\text{max}} P} \left( \frac{\mu^2}{6.1\mu - 7.5} \right) \quad (58)$$

Thus

$$L_{\text{mmHp}} = \frac{1}{\pi r^2} \frac{K_p + P}{\sigma \mu_{\text{max}} P} \left( \frac{\mu^2}{6.1\mu - 7.5} \right) \quad (59)$$

In terms of

$$L_{mmS} = \frac{1}{\pi r^2} \frac{K_S^2 + S^2}{\sigma \mu_{\max} S/X} \left( \frac{\mu^2}{6.1\mu - 7.5} \right)$$

In terms of Eckenfelder model

$$L_{ECm} = \frac{1}{\pi r^2} \left( \frac{\mu^2}{6.1\mu - 7.5} \right) \sigma K.S$$

In terms of mosers model

$$L_{mom} = \frac{1}{\pi r^2} \frac{K_S^2 + S^2}{\sigma \eta_{s \max} S^2} \left( \frac{\mu^2}{6.1\mu - 7.5} \right)$$

in terms of Miura's model

(60)

(61)

(62)

$$L_{min} = \frac{1}{\pi r^2} \frac{K_s^2 + S/X}{\sigma \eta_{smax} S/X} \left( \frac{\mu^2}{6.1\mu - 7.5} \right) \quad (63)$$

In terms of space time S(t)

$$S(t) = \frac{\mu_r}{fV_t} \quad (64)$$

In terms of space velocity S<sub>v</sub>

$$S_v = \frac{fV_t}{V_r} \quad (65)$$

In terms of heat generation per unit volume (R<sub>q</sub>) is given by

$$R_q = \frac{\Delta H_r F(t) X(t)}{V_r} \quad (66)$$

## Materials and Method

### Material

The following materials were used in carrying out the research work on the development of mathematical model for an adiabatic operation on biodegradation of petroleum hydrocarbon in plug flow reactor: Reactor, Filter, Petroleum hydrocarbon, Microbes, and Water

### Microbial Culture

Petroleum hydrocarbon from production terminal in Niger Delta area was collected. The microbes from the petroleum hydrocarbon were isolated and identified as pseudomonas species according to the method of (Buchaman & Gibbons 1974). A microbial culture was then prepared (pseudomonas species) for the research works.

### Determination of Microbial Concentration

One main experimental unit was set-up to generate the required data. The microbial concentration in the main experimental set-up was determined by counting the colony forming units/milliliter (cfu/ml) in a pour plate of mineral salt agar medium containing 0.5% petroleum hydrocarbon. Prior to this the pseudomonas species isolates had been inoculated aseptically into the main experimental unit set-up.

### Microbial Sample

Total microbial counts were measured by a standard plate count technique using difco plate count agar (APHA 1998).

## Results and Discussion

### Results

The developed model equations (59), (60) (61), (62) and (63) were computed and simulated with respect to reactor length and other functional parameters that determine the rate of reaction in a plug flow reactor. The following parameters were used  $\mu = 1.23(\text{hr}^{-1})$ ,  $K_p = K_s = 2.45\text{kg/m}^3$ ,  $\mu_{max} = 0.316$ ,

diameter  $d = 10.0\text{m}$ ,  $r = 5.0\text{m}$  ( $\rho = 1$ ),  $P = S = 0.35 - 0.95\text{kg/m}^3$ ,  $X = 0.2\text{kg/m}^3$ ,  $\mu_{max} = 0.316$

( $\text{hr}^{-1}$ )  $a=1$  and  $F_t = 100\text{kg/hr}$ .

The following results were obtained from the investigation. The results obtained are illustrated in Tables and figures as shown below;

**Table 1: Computational parameter of the different models**

Substrate Con. S (kg/m <sup>3</sup> )	J <sub>-eng</sub> Ji <sub>(m)</sub> <sub>__</sub>			
	<sup>^</sup> mmHp	J <sup>^</sup> mms	J <sup>^</sup> Ecm	~njgm
0.35	144.522	42.612	5.810	n2477926~~
0.45	114.408	37.094	6.185	246.154
0.55	96.826	33.566	7.559	239.328
0.65	84.674	31.138	8.934	229.110
0.75	75.814	29.357	10.308	216.100
0.85	68.919	27.985	!1.683	200.739
0.95	63.540	26.911	13.057	185.261

**Table 2: Computation of reactor volume at different substrate concentration for the various model's**

Substrate Con. S (kg/m <sup>3</sup> )	Reactor volume (m <sup>3</sup> )			
	* rmmHp	V mms	V <sub>Ecm</sub>	V mom
0.35	2270,441	669.435	75.565	3894.917
0.45	1797.350	582.747	97.166	3867.079
0.55	1521.136	527.322	318.752	3759.843
0.65	1330.229	489.178	140.353	3599.318
0.75	1191.038	461.198	161.939	3394.931
0.85	1082.717	439.644	183.540	3153.610
0.95	_99JU13___	422.772	205.125	2910.450

**Table 3: Computation of space time for the different model's at different substrate concentration for constant mass flow rate**

Substrate cone, (kg/m <sup>3</sup> )	Space time $\frac{V}{r}$ (IT)			
	S(t) <sub>mmHp</sub>	r <sub>(ti)Δr</sub>	S(t) <sub>aw,</sub>	S(t) <sub>mm</sub>
0.35	22.70	6.70	0.76	^T95~~
0.45	17.97	5.83	0.97	38.67
0.55	15.21	5.27	1.19	37.60
0.65	13.30	4.89	1.40	35.99
0.75	11.91	4.61	1.62	33.95
0.85	10.83	4.40	1.84	31.54
0.95	9.98	4.23	2.05	29.10

**Table 4: Computation of space velocity for the different model's at different substrate concentration for constant mass flow rate**

Substrate cone. (kg/m <sup>3</sup> )	Space velocity $\frac{r}{V}$ (V)			
	S(t) <sub>mmHp</sub>	Mvrms	S(t) <sub>Ecm</sub>	S(t) <sub>mm</sub>
0.35	0.044	0.149	1.316	fo026
0,45	0.056	0.172	1.031	0.026
0.55	0.066	0.190	0.840	0.027
0.65	0.075	0.204	0.714	0.028
0.75	0.084	0.217	0.617	0.029
0.85	0.092	0.227	0.543	0.032
0.95	0.100	0.236	0.488	0.034

**Table 5; Computation of reactor concentration**

**volume at different radius for 0.35kg/m<sup>3</sup> of substrate**

Radius (m)	Reactor volume (m <sup>3</sup> )				Substrate con. S kg/m <sup>3</sup>
	V <sub>mm</sub>	V <sub>mms</sub>	V <sub>recm</sub>	V <sub>mom</sub>	
6	16347	4820	544	28043	0.35
7	22256	6562	741	38181	
8	29049	8565	967	49833	
6	12941	4196	700952	27843	0.45
7	17619	5612	1243	37908	
8	22996	7456	49477		
6	10952	3797 5169	855	27071	0.55
7	14911	5212	1164	36857	
8	19462	7169	1519	48105	
6	9578	3522	1011	25915	0.65
7	13040	4795	1376	35283	
8	17019	6259	1796	46051	
6	8575	3321	1166	24444	0.75
7	11675	4521	1587	33279	
8	15239	5901	2072	43436	
6	7796	3165	1321	22706	0.85
7	10614	4310	1799	30914	
8	13853	5625	2348	40349	
6	7187	3044	1477	20955	0.95
7	9785	4144	2011	28530	
8	12771	5409	2624	37237	

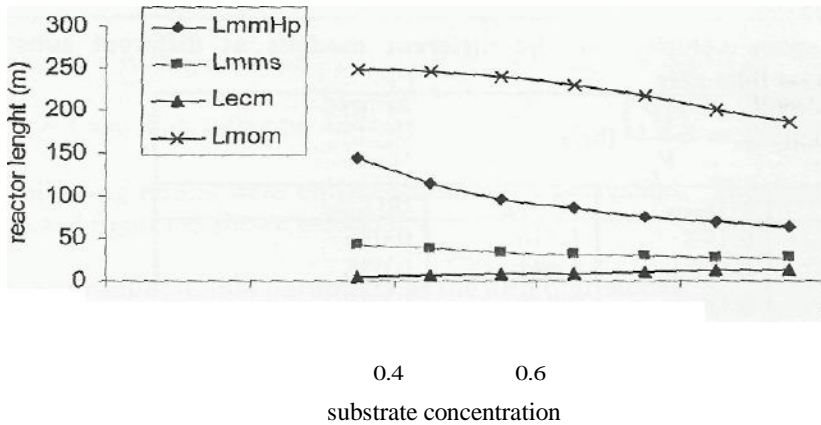
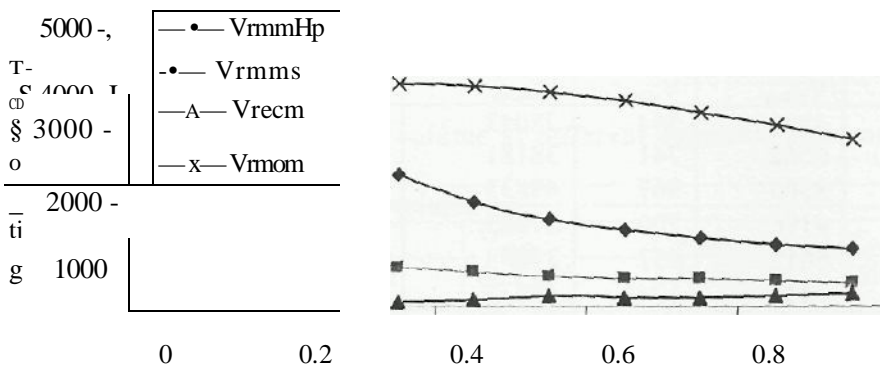


Figure 5.1: Reactor length versus substrate concentration



substrate concentration (kg/m)

Figure 5.2: React' volume versus substrate concentration

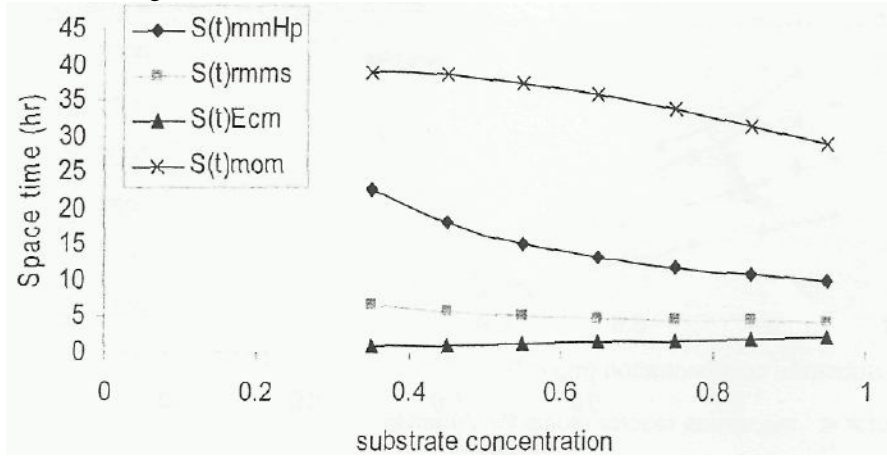


Figure 5.3: Space time versus substrate concentration

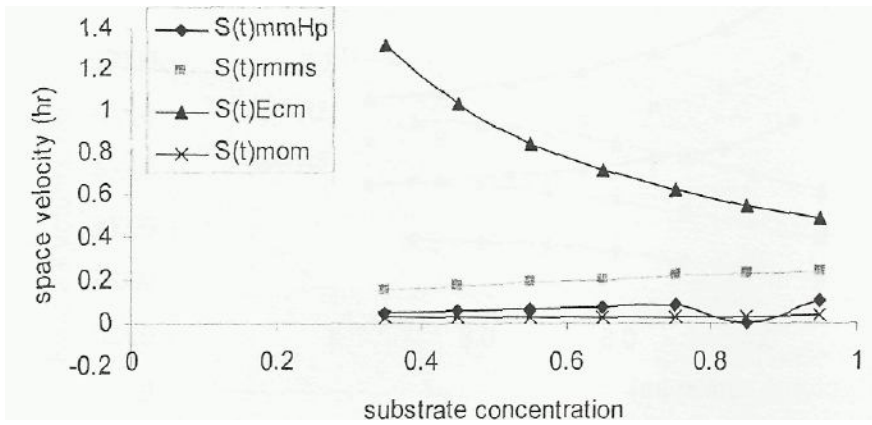


Figure 5.4: Space velocity versus substrate concentration

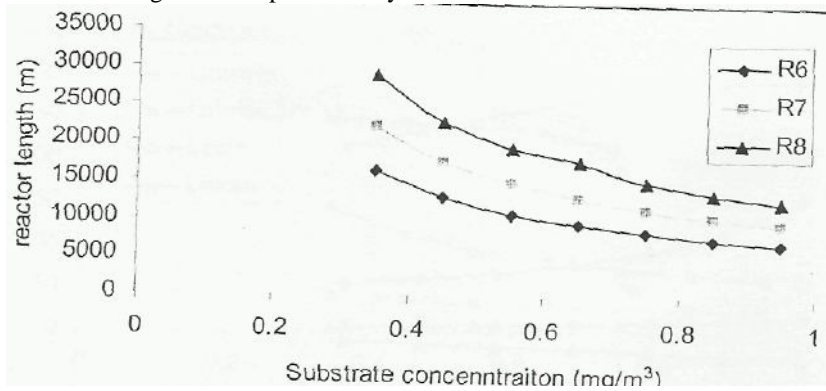
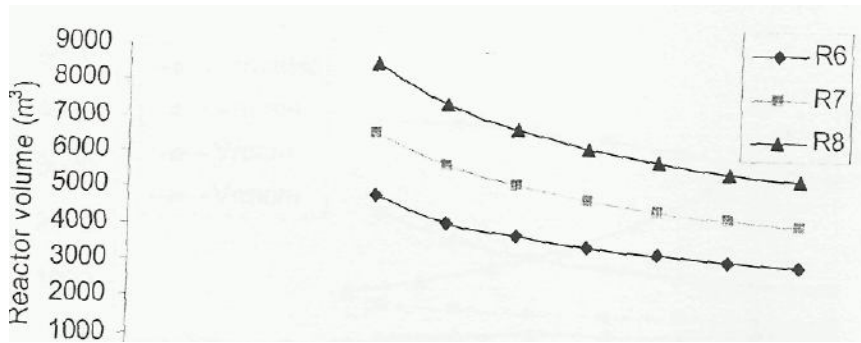


Figure 5.5: Reactor volume versus reactor radius for VrmmHp



radius (mj Figure 5.6: Reactor volume versus reactor radius for  $V_{rEcm}$

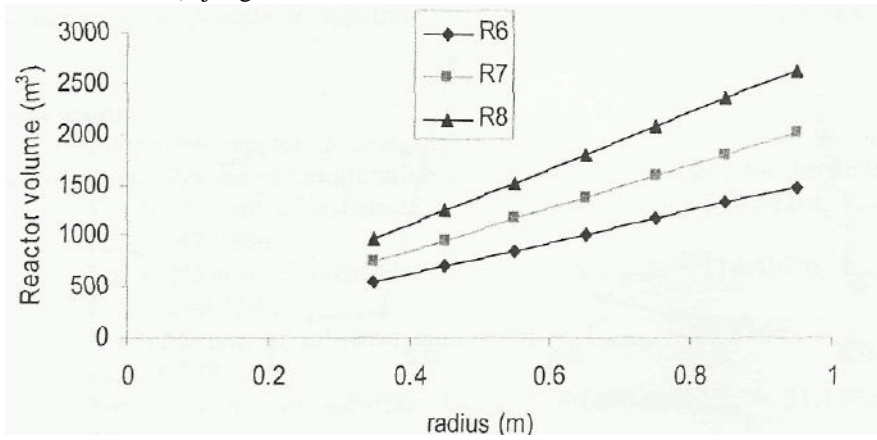


Figure 5.7: Reactor volume versus reactor radius for  $V_{rEcm}$

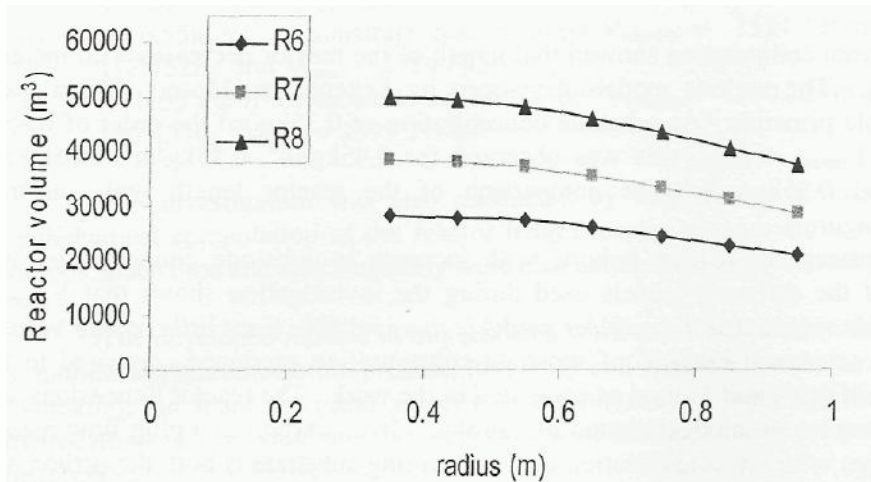


Figure 5.8: Reactor volume versus reactor radius for  $V_{rEcm}$

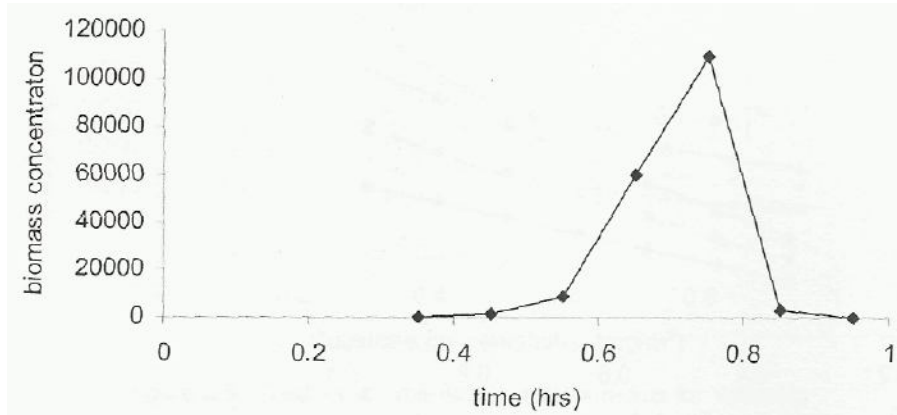


Figure 5.9 Biomass growth rate at different substrate concentration

### Discussion

Results obtained from computation showed that length of the reactor decreases with increase in substrate concentration. The various models developed by Eckenfelder, Mosers, Miura's and Monod followed the same principle. At substrate concentration of  $0.35\text{kg/m}^3$  the order of reactor length is  $L_{\text{Ecm}} < L_{\text{mms}} < L_{\text{mmHp}} < L_{\text{mom}}$ , this was observed for  $0.45\text{kg/m}^3$ ,  $0.55\text{kg/m}^3$ ,  $0.65\text{kg/m}^3$ ,  $0.75\text{kg/m}^3$ ,  $0.85\text{kg/m}^3$  and  $0.95\text{kg/m}^3$ . The comparison of the reactor length with substrate concentration is shown in figure 1.

From figure 2 decrease in reactor volume with increase in substrate concentration was observed. Comparison of the different models used during the investigation shows that  $V_{\text{rmon}} > V_{\text{rmmiip}} > V_{\text{rmmms}} > V_{\text{rEcm}}$ . This means that Eckenfelder model is more reliable since little reactor volume ( $75,656\text{m}^3$ ) is required to achieve  $0.35\text{kg/m}^3$  of substrate concentration produced compared to the reactor volumes of Moser, Miura's and Monod as computed in the work. The reactor dimensions as a function of the adiabatic process on biodegradation of petroleum hydrocarbon in a plug flow reactor was studied under the design with the consideration that the limiting substrate is both the carbon and energy source and hydrolysis is complete so that all petroleum hydrocarbon can be treated to yield carbon dioxide, heat, new biomass. The biomass growth rate was observed at the progressive phase. The result shows no lag phase, no stationary phase, but experienced death phase or decline, phase as shown in figure 9.

Computation of space time and space velocity for different models at different substrate concentration at constant mass flow rate was illustrated. The results obtained showed that increase in substrate concentration yields decrease in space time for the various model Monod, Mosers and Miura's and increase in Eckenfelder model as shown in Figure 3. Similarly, in terms of space velocity, its substrate concentration increase with increase in space time for Monod, Mosers and Miura's model and as well as decrease in Eckenfelder model as shown in Figure 4.

Computation of reactor volume at different radius for  $0.35\text{kg/m}^3$  to  $0.95\text{kg/m}^3$  of substrate concentration was investigated. Results obtained from the investigation shows decrease in reactor volume with increase in substrate concentration at a constant radius of 6, 7 and 8. These changes were obtained only for Monod, Mosers and Miura's model, whereas the Eckenfelder model was increasing with increase in substrate concentration at constant radius as shown in figures 5, 6, 7 and 8.

### Conclusion

Plug flow reactor is designed for the adiabatic operation on biodegradation of petroleum hydrocarbon. Results of computation gives volume of reactors for the different model as follows:

- (i) For  $0.35\text{kg/m}^3$  of substrate concentration,  $L_{\text{mmiip}}=144.522\text{m}$ ,  $L_{\text{mms}}=42.612\text{m}$ ,  $L_{\text{Rcm}}=4.810\text{m}$ ,  $L_{\text{mom}}=247,926\text{m}$
- (ii) For  $0.45\text{kg/m}$  of substrate concentration  $L_{\text{mmiip}} \sim 114.408\text{m}$ ,  $L_{\text{mms}}=37.094\text{m}$ ,  $L_{\text{Rcm}}=6.185\text{m}$ ,  $L_{\text{mom}}=246.154$ .
- (iii) For  $0.55\text{kg/m}$  of substrate concentration  $L_{\text{mmHp}} \sim 96.826\text{m}$ ,  $L_{\text{mms}} = 33.566\text{m}$ ,  $L_{\text{Ecm}} = 7.559\text{m}$ ,  $L_{\text{mom}} = 239,328\text{m}$
- (iv) For  $0.65\text{kg/m}^3$  of substrate  $L_{\text{mmHp}} = 84.675\text{m}$ ,  $L_{\text{mms}} = 31.138\text{m}$ ,  $L_{\text{Ecm}} = 8.934\text{m}$ ,  $L_{\text{mom}} -$



229.110m.

Similarly in terms of reactor volume

- (i) At 0.35kg/m<sup>3</sup> of substrate concentration  $V_{mmllp} = 2270.441m^3$ ,  $V_{rmmms} = 669.435m^3$ ,  $V_{rEcm} = 75.565m^3$  and  $V_{mom} = 3894.917m^3$ .
- (ii) At 0.45kg/m<sup>3</sup> of substrate concentration  $V_{mmMlp} = 1797.350m^3$ ,  $V_{rmmms} = 582.747m^3$ ,  $V_{rEcm} = 97.166m^3$  and  $V_{mom} = 3867.079ml$
- (iii) At 0.55kg/m<sup>3</sup> of substrate concentration  $V_{mmHlp} = 1521.136m^3$ ,  $V_{rmmms} = 5273.22m^3$ ,  $V_{rEcm} = 118.752m^3$  and  $V_{mom} = 3759.843m^3$
- (iv) At 0.65 kg/m<sup>3</sup> of substrate concentration  $V_{mmllp} = 1330.229m^3$ ,  $V_{rmmms} = 489.178m^3$ ,  $V_{rEcm} = 140.453m^3$ ,  $V_{mom} = 3599.318m^3$ .

The investigation was also conducted by considering different reactor diameter and the mathematical computation of the reactor length reactor volume etc were determined. Similarly the various space time and space velocity were also determined as presented in the research work.

The developed models in this research work can be applied in the following areas: as a guide in monitoring bioremediation process, to qualify and characterize the biomass built up in a bioreactor Estimating the space time and velocity of the bioreactor, predicting the performance of petroleum hydrocarbon utilize, studying the mechanisms of biodegradation of petroleum hydrocarbon and its metabolites.

### Nomenclature

$-r_c$	-	Rate of reaction of component C (mol/m <sup>3</sup> .hr)
K		Equilibrium constant
$C_A$		Concentration of component A (mol/m )
CB	-	Concentration of component B (mol/m <sup>3</sup> )
K <sub>1</sub>		Equilibrium constant for the rate of forward reaction
K <sub>2</sub>	-	Equilibrium constant for the rate of backward reaction
$d_m$	-	Change in mass of the slice bed (kg)
A	-	Reactant component of A
DI		Change in length of the slice bed (m)
R		Universal gas constant
T	-	Temperature °C
$\rho_s$		Density of the substrate (kg/m <sup>3</sup> )
$V_a$	-	Volume of a segment (m )
$X_c$		Fractional conversion of carbon
$X_{H2}$	-	Fractional conversion of hydrogen
$X_{cu3}$	-	Fractional conversion of methane
$X_{Air}$		Fraction conversion of air (oxygen)
Q	-	Heat in cal/kg.br
$R_A$	-	Rate of reaction (mol/m <sup>3</sup> .hr)
$X_A$	-	Fractional conversion of reactant A
$\mu$	-	Specific growth rate of microbes (cfu/ml.br)
S	-	Substrate concentration (mol%)
P		Product concentration (mol/m <sup>3</sup> .hr)
AHr	-	Enthalpy (k.cal/g)
$Y_s$	-	Yield coefficient (cell/g)
$Y_e$	-	Yield coefficient (cell/g of QI consumed)
$Y_i$		Yield factor (grain of cell mass per kilocalorie of heat evolved)
$T_s$	-	Specific rate (mol/m <sup>3</sup> .hr)
$\mu_{smax}$		Maximum specific rate (m <sup>3</sup> .hr/mol)
$V_{reactior}$	•	Volume of reactor (m)
L	-	Length of reactor (m)
D	-	Diameter of reactor (m)
R	-	Radius of reactor (m)
$Q_g$	-	Instantaneous microbial heat generated (Kcai/g)

$K_p$  - Equilibrium constant of the product (dimensionless)

### References

- Aiba S; Haung K.L., Moritz V, & Someya J.J. (1969). *Ferm. Technol. Journal of Biotechnology*, 47, p.21
- APHA (1989). American public health association public health and managed care. Washington D.C. (126<sup>th</sup> meeting), November, pp.15-19. -
- Brakstad, O., & Bonaunet, K. (2006), Biodegradation of Petroleum Hydrocarbon, *Journal of Biotechnology*, 17(2), pp.63-70.
- Buchaman R.E. & Gibbons N.E. (eds.) (1974). *Sergey's manual of determinative bacteriology*, 7th ed. Baltimori. The William and Whisking Co. p.274.
- Eade N. R, Taussing L. M., & Marks M.I. (2000), Hydrocarbon Pneumonitis. *Pediatrics*, pp. 351-357.
- Echoscan (2006). *Physical Properties of Hydrocarbon* [Online], hUp:l Imemebrs. Necon.org/echoscan 11
- Gerardet, P. Murray R.C.E. Cstillion R.W., Nester, E.W., Wood W.A., Krieg N.R. & Philips G.B. (1981). *Manual of Methods for General Bacteriology*. Washington D.C. (Amer Soc. Microbial), pp.30-90.
- Harms, H. & T. N. P. Bosnia (1997), Mass transfer limitation of microbial growth and pollutant degradation. *Journal of Ind. Microbial*, 6, (2), pp.97-105.
- Kinigoma I. B, (2002), Design of isothermal plug flow reactor for the manufacture of hydrochloric acid, *Journal of International Science and Engineering*. 7(2), pp.43-48.
- Litovitz, T. L. Schmitz, B. F., & Holm, K.C (1988). Annual report of the American association of poison control centers national data collection system [Online]. *Am Emerg Med* 1989, Sept. 7, pp. 495-545.
- Miura, Y (1978) In advances in biochemical engineering *Journal of Biotechnology*, 9 (31), pp. 62-70.
- Moo-Young M & Shimizu T. (1971). *Biotechnology, Journal of Bioengineering*, 13 (761), pp 101-112.
- Ophardt, C. E, (2003), *Virtual chembook, hydrocarbons*. Online] [http://www.elmlurjt.edu/chjiT/vchembook/501\\_hcboiling\\_pts.htm](http://www.elmlurjt.edu/chjiT/vchembook/501_hcboiling_pts.htm)
- Ott, L. (2007), *Plug flow reactor*, [OnLine],//A:PIug-Flow % 20 reactor.
- Renneboog R.M.J. (2006). *Uses of hydrocarbons*, (2002), [Online], [http://www.Scienceiq.com/show\\_fact.cfm](http://www.Scienceiq.com/show_fact.cfm).
- Sarkar D, Datta R. & Ferguson M. (2003). Biodegradation of petroleum hydrocarbons in soils, earth and environmental science department university of texas, San Antinio [Online], <http://84508.htm>.
- Taiwo A, (2001). *Fundamentals of chemical engineering thermodynamics*, 1<sup>s</sup> Ed, Osia publication, (S) Ohanda Street, Diobu Port Harcourt, Nig., pp. 10-100.
- Ukpaka C.P., Ogoni H. A., Amadi S. A. & Adebayo T. A. (2004). Mathematical modeling of the microbial growth and decay rate of pseudomonas sp on biodegradation of bonny light crude oil, *global Journal of Pure and Applied Sciences*, 11, (3), pp.423-431.

Vogel, R. H. & Ott, L. (2007). *Plug flow reactors*, [online], File://A: Conversion % 20 of % 20 Biomass % 20 in % 20 Supercritical % 20 Sluids. Htm.

Wikipedia, (2006). *Hydrocarbon* [online],[http:// wikipedia. Org/wiki/ Hydrocarbon](http://wikipedia.Org/wiki/Hydrocarbon).